

CENTER  
OVERVIEW

CELL  
MODELING

VIRUS &  
MOLECULAR  
MODELING

PERSONNEL

PUBLICATIONS

PRESENTATIONS

CONTACT US

## Publications

Jaqaman, K. and P. Ortoleva. 2002. New space warping method for the simulation of large-scale macromolecular conformational changes, *Journal of Computational Chemistry*, Vol 23(1), 484-491.

Tuncay, K. and P. Ortoleva. 2002. Probability functionals, homogenization and comprehensive reservoir simulators. Resource Recovery, Confinement, and Remediation of Environmental Hazards, Institute of Mathematics and its Applications volume 131, Editors: John Chadam, Al Cunningham, Richard E. Ewing, Peter Ortoleva, and Mary Fanett Wheeler, Springer-Verlag, New York, 161-178.

P. Ortoleva, E. Berry, Y. Brun, J. Fan, M. Fontus, A. Navid, A. Sayyed-Ahmad, Z. Shreif, F. Stanley, K. Tuncay, E. Weitzke and L. Wu. 2003. Karyote: physico-chemical genome, proteome, metabolome cell modeling system, *OMICS: A Journal of Integrative Biology*, Vol 7, 169-183.

Weitzke, E. and P. Ortoleva. 2003. Simulating cellular dynamics through a coupled transcription, translation, metabolic model, *Computational Biology and Chemistry*, Vol 27(4-5), 469-481.

Jaqaman, K., K. Tuncay and P. Ortoleva. Density functional theory of orientational order at interfaces: application to water, *Journal of Chemical Physics* (in press).

Sayyed-Ahmad, A., K. Tuncay and P. Ortoleva. 2003. Toward Automated Cell Model Development through Information Theory, *Journal of Physical Chemistry A* 107, 10554-10565.

Sayyed-Ahmad, A., Tuncay, K. and P. Ortoleva. 2003. Efficient solution Technique for Solving the Poisson-Boltzmann Equation, *Journal of Computational Chemistry* Vol 25: 1068-1074.

Fan, J., A. Navid, K. Tuncay and P. Ortoleva. 2004. Simulating multi-scale cellular reaction-transport processes, *Physical Review E* (in press).

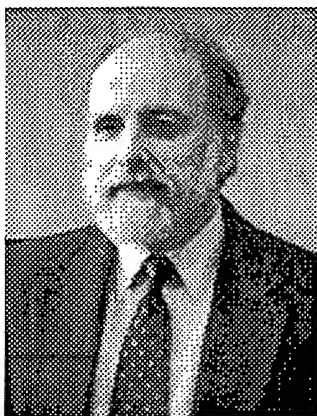
Navid, A. and P. Ortoleva. 2004. Simulated nonlinear dynamics of glycolysis in the protozoan parasite *Trypanosoma brucei*, *Journal of Theoretical Biology* (in press).

Tuncay, K., A. Sayyed-Ahmad, L. Jarymowycz and P. Ortoleva. Mesoscopic theory of multi-phase structures and macromolecule-fluid interactions, *Journal of Computational Chemistry* (submitted for publication).



People > Faculty > Peter Ortoleva

## Peter Ortoleva



### Professor, Geological Sciences and Chemistry

Theoretical Geochemistry

B.A., Rensselaer Polytechnic Institute

Ph.D. Cornell, 1970

phone: 812-855-2717

office: CH203E

E-mail

### Research

A unified approach to the modeling of a range of phenomena from intracrystalline zoning to basin diagenesis is adopted. The emphasis is on the challenging problem of strongly coupled systems.

Models are under development for oscillatory and sector crystal zoning, differentiated diagenetic and metamorphic layering, stylolites, banded and mosaic agates and temporally oscillatory fluid migration in sedimentary basins.

Petroleum and mineral exploration is being facilitated by the development of a basin diagenesis code which accounts for a complete suite of mechanical, reaction and transport processes. The code is used to predict the distribution of diagenetic and structural petroleum traps within the basin and the development of over- and under-pressures in reservoir rock. Another code focuses on the imposition of reactive fluids on a rock over geological or engineering time scales.

This research is supported by grants from the US DOE, Gas Research Institute, NSF, the EPA and the petroleum and computer industries. The Indiana University Laboratory for Computational Geochemistry under Ortoleva's supervision provides an interdisciplinary research environment and supports about 15 graduate and postdoctoral students from computer science, chemistry, geology, mathematics and physics, one half being from the Department of Geological Sciences.

### Representative Publications

Meshri, I. and P. Ortoleva, eds., Prediction of Reservoir quality through chemical modeling: (1990). AAPG Memoir 49, 175p.

Ortoleva, P., B. Hallet, A. McBirney, I. Meshri, R. Reeder, and P. Williams, eds., Self-organization in geological systems: (1990). Proceedings of a workshop held 26-30 June 1988, University of California, Santa Barbara. Earth Science Reviews 29, Amsterdam, Elsevier, 417p.

Ortoleva, P., Nonlinear chemical waves: (1992). Chichester, John Wiley and Sons, 302p.

Ortoleva, P., Geochemical self-organization: (1994). Oxford University Press, 411p.

Ortoleva, P., Basin Compartments and Seals: (1994). AAPG Memoir 61, 477p.

## Student Theses

Dewers, Thomas A. (Ph.D., 1990) Non-linear dynamics of coupled water-rock reaction, transport, and rock deformation.

Chen, Yueting (Ph.D., 1994) CIRF.A: a general, coupled reaction-transport model and simulator.

Payne, Dorothy F. (M.Sc., 1995) The effect of reaction-transport-mechanical processes on the spatial and temporal evolution of diagenetic phenomena in sedimentary basins: a test of the CIRFB code.

Sakrani, Khairiddine (Ph.D., 1996) A unified texture and mineralogy dependent model for rock deformation.

[★ BACK TO TOP](#)

### INDIANA UNIVERSITY DEPARTMENT OF GEOLOGICAL SCIENCES

1001 East 10th Street  
Bloomington, IN 47405-1405  
Phone 812-855-5582 | Fax 812-855-7899  
[Contact Us](#)

[Search Site](#)  
Last updated: 11 Aug 2004  
Copyright 2004, The Trustees of [Indiana University](#)  
[Copyright Complaints](#)

# Faculty Publications

Chemistry Department

Indiana University  
Bloomington

## Peter J. Ortoleva

### Year-wise listing of Publications:

[2002](#)[2001](#)[2000](#)

#### 2002

- Jaqaman, K. and Ortoleva, P. J. (2002). "New space warping method for the simulation of large-scale macromolecular conformational changes." Journal of Computational Chemistry **23**(4): 484-491.

[top](#)

#### 2001

- Payne, D. F. and Ortoleva, P. J. (2001). "A model for lignin alteration - part II: numerical model of natural gas generation and application to the Piceance Basin, Western Colorado." Org. Geochem. **32**(9): 1087-1101.
- Payne, D. F. and Ortoleva, P. J. (2001). "A model for lignin alteration - part I: a kinetic reaction-network model." Org. Geochem. **32**(9): 1073-1085.
- Tuncay, K. and Ortoleva, P. (2001). "Salt tectonics as a self-organizing process: a reaction, transport, and mechanics model." J. Geophys. Res., [Solid Earth] **106**(B1): 803-817.

[top](#)

#### 2000

- Ozkan, G. and Ortoleva, P. (2000). "A mesoscopic model of nucleation and Ostwald ripening/stepping. Application to the silica polymorph system." J. Chem. Phys. **112**(23): 10510-10525.
- Payne, D. F., Tuncay, K., Park, A., Comer, J. B. and Ortoleva, P. (2000). "A reaction-transport-mechanical approach to modeling the interrelationships among gas generation, overpressuring, and fracturing: implications for the Upper Cretaceous natural gas reservoirs of the Piceance Basin, Colorado." AAPG Bull. **84**(4): 545-565.

[top](#)

---

[| Home | Browse Publications | Help | Contact |](#)

Last Updated: April 2, 2002

Send Comments to: [Gary Wiggins](#)Copyright © 2001-2002 The Trustees of [Indiana University](#)

dblp.uni-trier.de

# Peter J. Ortoleva

List of publications from the [DBLP Bibliography Server](#) - [FAQ](#)

[Coauthor Index](#) - Ask others: [ACM DL](#) - [ACM Guide](#) - [CiteSeer](#) - [CSB](#) - [Google](#)

2004		
3	EE	Abdallah Sayyed-Ahmad, Kagan Tuncay, Peter J. Ortoleva: Efficient solution technique for solving the Poisson-Boltzmann equation. <i>Journal of Computational Chemistry</i> 25(8): 1068-1074 (2004)
2003		
2	EE	Elizabeth L. Weitzke, Peter J. Ortoleva: Simulating cellular dynamics through a coupled transcription, translation, metabolic model. <i>Computational Biology and Chemistry</i> 27(4-5): 469-480 (2003)
2002		
1	EE	Khuloud Jaqaman, Peter J. Ortoleva: New space warping method for the simulation of large-scale macromolecular conformational changes. <i>Journal of Computational Chemistry</i> 23(4): 484-491 (2002)

## Coauthor Index

1	Khuloud Jaqaman	[1]
2	Abdallah Sayyed-Ahmad	[3]
3	Kagan Tuncay	[3]
4	Elizabeth L. Weitzke	[2]

DBLP: [[Home](#) | [Search: Author, Title](#) | [Conferences](#) | [Journals](#)]

*Michael Ley (ley@uni-trier.de) Thu Aug 25 20:20:16 2005*